CONFORMATIONAL STUDY OF DIBENZYL ETHER

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Understanding the initial stages of polycyclic aromatic hydrocarbon (PAH) aggregation, the onset of soot formation, is an important goal on the pathway to cleaner combustion processes. PAHs with short alkyl chains, present in fuel-rich combustion environments, can undergo reactions that will chemically link aromatic rings together. One such example of a linked diaryl compound is dibenzyl ether, C_6H_5-CH_2-O-CH_2-C_6H_5. The –CH_2-O-CH_2- linkage has a length and flexibility well-suited to forming a π-stacked conformation between the two phenyl rings. In this talk, we will explore the single-conformation spectroscopy of dibenzyl ether under jet-cooled conditions in the gas phase. Laser-induced fluorescence, chirped pulse Fourier transform microwave (8-18 GHz region), and single-conformation infrared spectroscopy in the alkyl CH stretch region were all carried out on the molecule, thereby interrogating its full array of electronic, vibrational and rotational degrees of freedom. This work is the first step in a broader study to determine the extent of π-stacking in linked aryl compounds as a function of linkage and PAH size.